



# wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 4DO2  
Title : Crystal Structure of the Rop protein mutant D30P/A31G at resolution 1.4 resolution.  
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Deposited on : 2012-02-09  
Resolution : 1.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

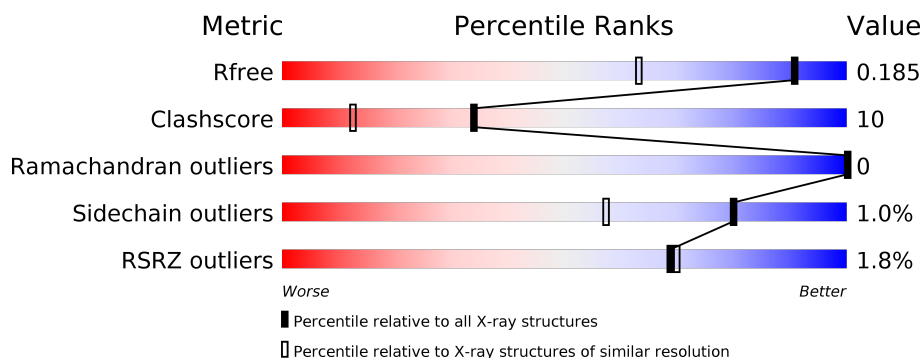
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1307 (1.40-1.40)
Clashscore	112137	1411 (1.40-1.40)
Ramachandran outliers	110173	1373 (1.40-1.40)
Sidechain outliers	110143	1372 (1.40-1.40)
RSRZ outliers	101464	1315 (1.40-1.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	70	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; text-align: center;">%</div> <div style="position: absolute; top: 10px; left: 0; width: 100%; text-align: center;"> <span style="display: inline-block; width: 69%; height: 10px; background-color: green;"></span> <span style="display: inline-block; width: 11%; height: 10px; background-color: yellow;"></span> <span style="display: inline-block; width: 19%; height: 10px; background-color: grey;"></span> </div> </div> </div>
1	B	70	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; text-align: center;">%</div> <div style="position: absolute; top: 10px; left: 0; width: 100%; text-align: center;"> <span style="display: inline-block; width: 71%; height: 10px; background-color: green;"></span> <span style="display: inline-block; width: 10%; height: 10px; background-color: yellow;"></span> <span style="display: inline-block; width: 19%; height: 10px; background-color: grey;"></span> </div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1102 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Regulatory protein rop.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	57	Total	C	N	O	S	0	6	0
			468	287	82	95	4			
1	B	57	Total	C	N	O	S	0	6	0
			465	286	82	93	4			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	PRO	ASP	ENGINEERED MUTATION	UNP P03051
A	31	GLY	ALA	ENGINEERED MUTATION	UNP P03051
A	64	GLU	-	EXPRESSION TAG	UNP P03051
A	65	HIS	-	EXPRESSION TAG	UNP P03051
A	66	HIS	-	EXPRESSION TAG	UNP P03051
A	67	HIS	-	EXPRESSION TAG	UNP P03051
A	68	HIS	-	EXPRESSION TAG	UNP P03051
A	69	HIS	-	EXPRESSION TAG	UNP P03051
A	70	HIS	-	EXPRESSION TAG	UNP P03051
B	30	PRO	ASP	ENGINEERED MUTATION	UNP P03051
B	31	GLY	ALA	ENGINEERED MUTATION	UNP P03051
B	64	GLU	-	EXPRESSION TAG	UNP P03051
B	65	HIS	-	EXPRESSION TAG	UNP P03051
B	66	HIS	-	EXPRESSION TAG	UNP P03051
B	67	HIS	-	EXPRESSION TAG	UNP P03051
B	68	HIS	-	EXPRESSION TAG	UNP P03051
B	69	HIS	-	EXPRESSION TAG	UNP P03051
B	70	HIS	-	EXPRESSION TAG	UNP P03051

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	96	Total	O	0	0
			96	96		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	73	Total	O	0	0
			73	73		



- Molecule 1: Regulatory protein rop



- Molecule 1: Regulatory protein rop



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	26.67Å 38.82Å 56.64Å 90.00° 100.87° 90.00°	Depositor
Resolution (Å)	55.64 – 1.40 18.54 – 1.40	Depositor EDS
% Data completeness (in resolution range)	99.0 (55.64-1.40) 99.0 (18.54-1.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.38 (at 1.40Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.159 , 0.188 0.155 , 0.185	Depositor DCC
$R_{free}$ test set	1142 reflections (5.40%)	DCC
Wilson B-factor (Å <sup>2</sup> )	13.0	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 43.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	1102	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 54.19 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.7871e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	1.21	0/510	1.22	4/681 (0.6%)
1	B	1.32	0/500	1.26	4/669 (0.6%)
All	All	1.27	0/1010	1.24	8/1350 (0.6%)

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	43	ASP	CB-CG-OD2	7.15	124.74	118.30
1	A	16	ARG	NE-CZ-NH2	-6.91	116.84	120.30
1	A	55	ARG	NE-CZ-NH2	-6.63	116.98	120.30
1	B	32	ASP	CB-CG-OD1	6.44	124.09	118.30
1	A	36	ASP	CB-CG-OD2	-6.20	112.72	118.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	468	0	453	16	0
1	B	465	0	449	2	0
2	A	96	0	0	2	0
2	B	73	0	0	2	0
All	All	1102	0	902	18	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

The worst 5 of 18 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11[B]:MET:HE3	2:B:173:HOH:O	1.25	1.30
1:A:3[A]:LYS:HZ3	1:A:6[A]:LYS:NZ	1.42	1.16
1:A:3[A]:LYS:NZ	1:A:6[A]:LYS:HZ2	1.49	1.10
1:A:3[A]:LYS:NZ	1:A:6[A]:LYS:NZ	2.15	0.82
1:A:39:GLU:OE1	2:A:188:HOH:O	2.12	0.66

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	61/70 (87%)	60 (98%)	1 (2%)	0	100	100
1	B	60/70 (86%)	59 (98%)	1 (2%)	0	100	100
All	All	121/140 (86%)	119 (98%)	2 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	56/62 (90%)	54 (96%)	2 (4%)	40 9
1	B	54/62 (87%)	54 (100%)	0	100 100
All	All	110/124 (89%)	108 (98%)	2 (2%)	80 30

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11[A]	MET
1	A	11[B]	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	57/70 (81%)	-0.40	1 (1%) 69 70	9, 14, 25, 33	2 (3%)
1	B	57/70 (81%)	-0.29	1 (1%) 69 70	8, 13, 25, 39	0
All	All	114/140 (81%)	-0.35	2 (1%) 69 70	8, 13, 25, 39	2 (1%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	57	GLY	5.1
1	A	57	GLY	3.8

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.